



ELSEVIER

Discrete Applied Mathematics 121 (2002) 295–306

DISCRETE
APPLIED
MATHEMATICS

Ordering graphs with small index and its application

Fuji Zhang^{a, 1}, Zhibo Chen^{b,*, 2}

^a*Department of Mathematics, Xiamen University, Xiamen 361005, China*

^b*Department of Mathematics, Penn State University, McKeesport, PA 15132, USA*

Received 7 January 2000; received in revised form 1 May 2001; accepted 25 June 2001

Abstract

We consider the problem of ordering connected graphs by index (the largest eigenvalue). The asymptotic ordering for the connected graphs with index less than $\sqrt{2 + \sqrt{5}}$ is determined. Its application to the study of acyclic Kekulean molecules with big HOMO–LUMO separation is also given. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Graph eigenvalue; Graph index; Acyclic Kekulean molecule; HOMO–LUMO separation

1. Introduction

The study of graph eigenvalues have long been attracting researcher's attention, and there are several monographs and a lot of research papers published continually (see [3,6,7,10] and their cited references). The study in this field is stimulated by a variety of problems in theoretical chemistry, quantum mechanics and statistical physics. On the other hand it also is closely related to many other areas of mathematics including spectral Riemannian geometry.

All graphs in this paper are finite and have no loops or multiple edges. The largest eigenvalue of the adjacency matrix of a graph G is called the index of G . The study of ordering graphs by index was first started by Collatz and Sinogowitz [4] in 1957. For trees with n vertices, Lovasz and Pelican [16] determined the extreme cases by proving that the star $K_{1,n-1}$ has largest index ($\sqrt{n-1}$) and the path P_n has smallest index ($2 \cos(\pi/(n+1))$). In 1979, Li and Feng [15] first raised the following problem. When a graph G is under some modification, its index changes correspondingly. Can

* Corresponding author.

E-mail address: zxc4@psu.edu (Z. Chen).

¹ Research supported by NSFC.

² Research supported in part by the RDG grant from the Penn State University.

we find the inherent relationship? In the same paper they gave two useful theorems each of which compares the indices of a graph and its certain modification. Since then the concept of graph perturbations was developed to study the effects of graph modifications to the graph spectrum. The study in this area has made great progress. For details, the reader is referred to the surveys [9,17] and the book [10]. In particular, most results up to the year 1989 were surveyed in [9], and one section of this survey is focused on the ordering of graphs by index. The most recent progress in this aspect is that Hofmeister [14] determined the ordering of the six trees with larger index and the further work of An Chang in his Ph.D. Thesis (Sichuan University, 1998).

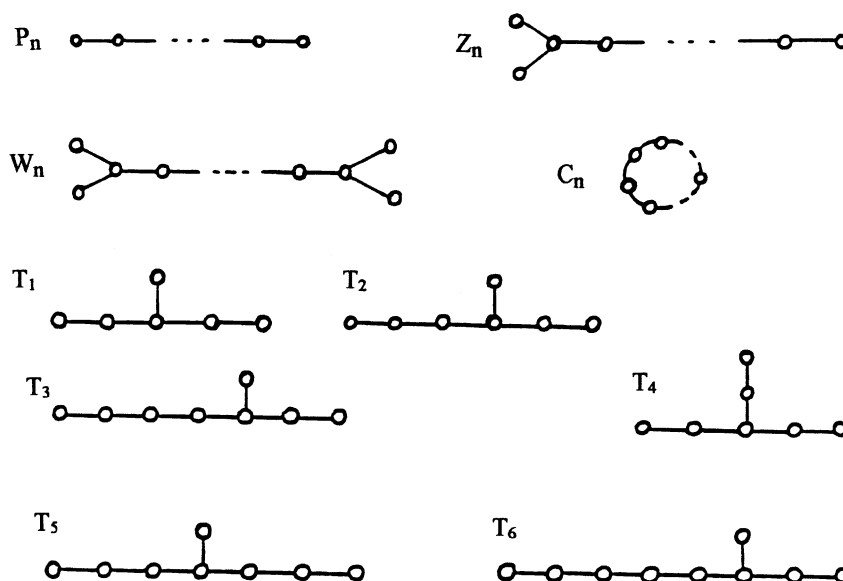
Our aim here is to study the ordering of graphs with small index. The asymptotic ordering of graphs with index less than $\sqrt{2 + \sqrt{5}}$ is determined in this paper. It should be noted that the ordering is for graphs with same number of vertices. We shall also reveal an interesting phenomenon that there are infinitely many pairs of sequences of graphs with index less than $\sqrt{2 + \sqrt{5}}$ having the following property: for each such pair there is a threshold value N such that the inequality comparing the indices of two graphs with same vertex number n but in different graph sequences changes its direction when and only when n passes N . Because of this phenomenon we can obtain some asymptotic comparison theorems and raise some research problem about the relative threshold function.

Now let us explain the reason why we only consider the graphs with index less than $\sqrt{2 + \sqrt{5}}$. Hoffman [12] studied limit points of graph indices, and he determined all limit points less than $\sqrt{2 + \sqrt{5}}$ and showed that these limit points approaches $\sqrt{2 + \sqrt{5}}$. He also suggested that possibly there exists a real number λ such that every number at least λ is a limit point of graph indices. In fact this is true with $\lambda = \sqrt{2 + \sqrt{5}}$, as proved by Shearer [19]. From this fact we see that the graph indices greater than $\sqrt{2 + \sqrt{5}}$ are dense and so they are hard to handle in view of ordering. It must also be noted that apart from cycles all the connected graphs with index at most $\sqrt{2 + \sqrt{5}}$ are trees.

2. Preparation

To give our main results we need the following lemmas. Let G be a simple graph with adjacency matrix A . The characteristic polynomial of G is $\chi(G, x) = |xI - A|$, where I denotes the identity matrix. The largest root of the characteristic polynomial of G is denoted by $\rho(G)$ and called the index of G .

Lemma 1 (Li and Feng [15], also see Cvetković et al. [10]). *Let G be a nontrivial connected graph and u a vertex of G . For non-negative integers k and l , let $G(k, l)$ denote the graph obtained from G by attaching pendant paths of lengths k and l at u . If $k \geq l \geq 1$, then $\chi(G(k, l), x) < \chi(G(k + 1, l - 1), x)$ for $x \geq \rho(G(k + 1, l - 1))$. In particular, $\rho(G(k, l)) > \rho(G(k + 1, l - 1))$.*

Fig. 1. Ω_1 : Graphs with index less than or equal to 2.

Lemma 2 (Hoffman and Smith [13], also see Cvetković et al. [10]). *Let G be a connected graph and let G_{uv} be obtained from G by subdividing the edge uv of G . If uv lies on an internal path of G , and if G is not isomorphic to W_n (as depicted in Fig. 1), then $\rho(G_{uv}) < \rho(G)$.*

Lemma 3 (Smith [20]). *The connected graphs whose index does not exceed 2 are precisely the graphs: P_n ($n \geq 1$), Z_n ($n \geq 3$), C_n ($n \geq 3$), W_n ($n \geq 5$), and T_i ($i = 1, 2, \dots, 6$), as depicted in Fig. 1.*

Note: The set of these graphs is denoted as Ω_1 , which includes the Dykin graphs ($\rho(G) < 2$) and the Euclid graphs ($\rho(G) = 2$).

Lemma 4 (Brouwer et al. [2], Cvetković et al. [5], Cvetković and Rowlinson [9]). *The connected graphs with index in the interval $(2, \sqrt{2} + \sqrt{5})$ are precisely the trees of the following types, as depicted in Fig. 2 :*

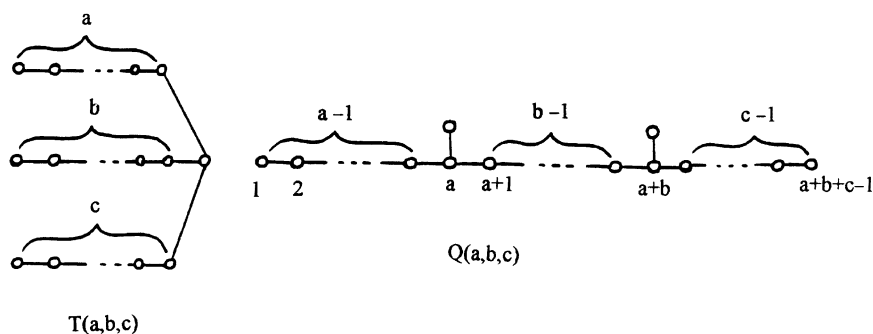
(a) $T(a, b, c)$ for

$$a = 1, b = 2, c > 5 \text{ or}$$

$$a = 1, b > 2, c > 3 \text{ or}$$

$$a = 2, b = 2, c > 2 \text{ or}$$

$$a = 2, b = 3, c = 3.$$

Fig. 2. Ω_2 : Graphs with index $\in (2, \sqrt{2 + \sqrt{5}})$.

- (b) $Q(a, b, c)$ for $(a, b, c) \in \{(2, 1, 3), (3, 4, 3), (3, 5, 4), (4, 7, 4), (4, 8, 5)\}$ or $a > 1$, $b \geq b^*(a, c)$, $c > 1$ where $(a, c) \neq (2, 2)$ and

$$b^*(a, c) = \begin{cases} a + c & \text{for } a > 3, \\ 2 + c & \text{for } a = 3, \\ -1 + c & \text{for } a = 2. \end{cases}$$

Here $T(a, b, c)$ denotes the tree with a vertex v of degree 3 such that $T(a, b, c) - v = P_a \cup P_b \cup P_c$, (where P_m denotes a path with m vertices) and $Q(a, b, c)$ denotes the tree obtained from the path with vertices $1, 2, \dots, a + b + c - 1$ (in order) by attaching a pendant edge at each of the vertices a and $a + b$.

(The set of these graphs is denoted as Ω_2 .)

The next lemma is essentially due to Hoffman [12]. The present form can be found in [11].

Lemma 5 (Hoffman). Let v_q be the largest real root of the polynomial

$$L_q(v) = v^q - (v^{q-2} + v^{q-3} + \dots + v + 1).$$

We set

$$\lambda_q = v_q^{1/2} + v_q^{-1/2}, \quad \text{and} \quad \lambda_\infty = v_\infty^{1/2} + v_\infty^{-1/2}.$$

Then $1 = v_2 < v_3 < \dots < v_q < v_{q+1} < \dots < v_\infty = \frac{1}{2}(\sqrt{5} + 1) \approx 1.618034$.

$$2 = \lambda_2 < \lambda_3 < \dots < \lambda_q < \lambda_{q+1} < \dots < \lambda_\infty = \sqrt{2 + \sqrt{5}} \approx 2.058171.$$

Moreover, for $c \geq 2$

$\rho(T(1, b, c))$ increases strictly with b and converges to λ_{c+1} ,

$\rho(T(2, b, 2))$ increases strictly with b and converges to λ_∞ ;

for $c \geq 3$ and a with $2 \leq a \leq c$,

$\rho(Q(a, b, c))$ decreases strictly with b and converges to λ_c .

The next lemma is a well known result from the theory of non-negative matrices.

Lemma 6 (See Cvetković et al. [7] Theorem 0.7). *The increase of any element of a non-negative matrix A does not decrease the greatest eigenvalue of A . The greatest eigenvalue increases strictly if A is an irreducible matrix. Therefore, in a connected graph G whose edges are assigned non-negative weights, every proper subgraph has the index smaller than the index of G .*

3. Main results

From Lemma 3 it is not difficult to give the ordering by index for the graphs with index not greater than 2, since we have known (cf. [8]) all the indices for these graphs: $\rho(P_n) = 2 \cos \pi/(n+1)$, $\rho(Z_n) = 2 \cos \pi/2(n-1)$ ($n \geq 3$), $\rho(C_n) = 2$ ($n \geq 3$), $\rho(W_n) = 2$ ($n \geq 5$), $\rho(T_1) = 2 \cos \pi/12$, $\rho(T_2) = 2 \cos \pi/18$, $\rho(T_3) = 2 \cos \pi/30$, $\rho(T_4) = \rho(T_5) = \rho(T_6) = 2$. When neglecting the few cases with $n \leq 10$, we have the ordering (see [21]) as

$$\rho(P_n) < \rho(Z_n) < \rho(W_n) = \rho(C_n) \quad \text{for } n > 10 \quad (*)$$

So we only need consider the graphs with index in the interval $(2, \sqrt{2 + \sqrt{5}})$. From Lemma 4, these graphs are precisely the two types of trees $T(a, b, c)$ and $Q(a, b, c)$ as depicted in Fig. 2. Since the indices of all trees with vertex number not exceeding 10 are listed in [7], we may restrict our attention to the trees with vertex number $n > 10$ in the following.

First we give the ordering for the first type of trees $T(a, b, c)$ with vertex number $n > 10$. We may assume $a \leq b \leq c$ without loss of generality.

Theorem 1. *When $n > 10$, we have*

$$\begin{aligned} \rho(T(1, 2, n-4)) &< \rho(T(1, 3, n-5)) < \dots < \\ &< \rho(T(1, \lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)) < \rho(T(2, 2, n-5)). \end{aligned}$$

Proof. All the inequalities except the last one immediately follow from Lemma 1. To prove the last inequality we first show the following two equalities:

$$\chi(T(2, 2, k), \lambda) = \chi(P_2, \lambda) \chi(\phi_{k+3}, \lambda), \quad (1)$$

$$\chi(T(k, k, 1), \lambda) = \chi(P_k, \lambda) \chi(\phi_{k+2}, \lambda), \quad (2)$$

where P_i is a path with i vertices, and ϕ_i is obtained from a path $v_1 v_2 \dots v_i$ by assigning a weight $\sqrt{2}$ to the edge $v_2 v_3$. Since the proof for the two equalities are similar, here

we only give the proof for the equality (1). It is clear that the characteristic polynomial $\chi(T(2,2,k), \lambda)$ is an $n \times n$ determinant where $n = k + 5$, since the tree $T(2,2,k)$ has $k + 5$ vertices. In fact,

$$\chi(T(2,2,k), \lambda) = \begin{vmatrix} \lambda & -1 & & & & & & & & & \\ -1 & \lambda & & & & & & & & & \\ & & \lambda & -1 & & & & & & & \\ & & -1 & \lambda & -1 & & & & & & \\ & -1 & & -1 & \lambda & -1 & & & & & \\ & & & -1 & \lambda & -1 & & & & & \\ & & & & & \cdot & \cdot & \cdot & & & \\ & & & & & & \cdot & \cdot & \cdot & & \\ & & & & & & & \cdot & \cdot & \cdot & \\ & & & & & & & & -1 & \lambda & -1 \\ & & & & & & & & -1 & \lambda & \end{vmatrix}_{n \times n}.$$

By elementary row operations adding (-1) Row 3 to Row 1 and adding (-1) Row 4 to Row 2, followed by column operations adding Col 1 to Col 3 and adding Col 2 to Col 4, the determinant becomes

$$\begin{vmatrix} \lambda & -1 & & & & & & & & & \\ -1 & \lambda & & & & & & & & & \\ & & \lambda & -1 & & & & & & & \\ & & -1 & \lambda & -1 & & & & & & \\ & -1 & & -2 & \lambda & -1 & & & & & \\ & & & -1 & \lambda & -1 & & & & & \\ & & & & \cdot & \cdot & \cdot & & & & \\ & & & & & \cdot & \cdot & \cdot & & & \\ & & & & & & \cdot & \cdot & \cdot & & \\ & & & & & & & -1 & \lambda & -1 & \\ & & & & & & & -1 & \lambda & \end{vmatrix}_{n \times n}.$$

Then by Laplace expansion we see that it equals

$$\begin{vmatrix}
 \lambda & -1 & & & & & & & & & \\
 -1 & \lambda & -\sqrt{2} & & & & & & & & \\
 & -\sqrt{2} & \lambda & -1 & & & & & & & \\
 & & -1 & \lambda & -1 & & & & & & \\
 & & & -1 & \lambda & -1 & & & & & \\
 & & & & -1 & \lambda & -1 & & & & \\
 & & & & & \cdot & \cdot & \cdot & & & \\
 & & & & & & \cdot & \cdot & \cdot & & \\
 & & & & & & & \cdot & \cdot & \cdot & \\
 & & & & & & & & -1 & \lambda & -1 \\
 & & & & & & & & -1 & \lambda & \\
 & & & & & & & & & & (n-2) \times (n-2)
 \end{vmatrix}$$

$$= \chi(P_2, \lambda) \chi(\phi_{n-2}, \lambda) = \chi(P_2, \lambda) \chi(\phi_{k+3}, \lambda). \text{ This proves (1).}$$

Now we use the two equalities to prove the last inequality in Theorem 1. We distinguish the two cases depending on the parity of n .

Case 1: n is even. Then $\lfloor (n-2)/2 \rfloor = \lceil (n-2)/2 \rceil = (n-2)/2$. From equalities (1) and (2) we see that when $n > 10$

$$\chi(T(2, 2, n-5), \lambda) = \chi(P_2, \lambda) \chi(\phi_{n-2}, \lambda),$$

$$\begin{aligned}
 \chi\left(T\left(1, \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right), \lambda\right) &= \chi\left(T\left(\frac{n-2}{2}, \frac{n-2}{2}, 1\right), \lambda\right) \\
 &= \chi(P_{\frac{n-2}{2}}, \lambda) \chi(\phi_{\frac{n+2}{2}}, \lambda).
 \end{aligned}$$

Note that the largest root of the product of two polynomials is the larger one between the largest roots of the two polynomials. Then by Lemma 6 we have

$$\rho\left(T\left(1, \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right)\right) = \rho(\phi_{\frac{n+2}{2}}) < \rho(\phi_{n-2}) = \rho(T(2, 2, n-5)).$$

Case 2: n is odd. Then $\lfloor (n-2)/2 \rfloor = (n-3)/2$, $\lceil (n-2)/2 \rceil = (n-1)/2$. Similar to case 1, when $n > 10$ we have

$$\chi\left(T\left(1, \frac{n-1}{2}, \frac{n-1}{2}\right), \lambda\right) = \chi(P_{\frac{n-1}{2}}, \lambda) \chi(\phi_{\frac{n+3}{2}}, \lambda),$$

so that

$$\begin{aligned} \rho\left(T\left(1, \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right)\right) &< \rho\left(T\left(1, \frac{n-1}{2}, \frac{n-1}{2}\right)\right) \\ &= \rho(\phi_{\frac{n+3}{2}}) < \cdots < \rho(\phi_{n-2}) = \rho(T(2, 2, n-5)). \end{aligned}$$

It completes the proof for Theorem 1. \square

The next theorem gives the ordering by index for the second type of trees $Q(a, b, c)$. Note that we may assume $a \leq c$ without loss of generality.

Theorem 2. When $n \geq 3k$, $k > 2$, we have

$$\rho(Q(2, n-k-3, k)) < \rho(Q(3, n-k-4, k)) < \cdots < \rho(Q(k, n-2k-1, k)).$$

Proof. We only need to prove $\rho(Q(a, b, c)) < \rho(Q(a+1, b-1, c))$ for $a, c > 1$, $b > a$. By Lemma 6, $\rho(Q(a, b, c)) < \rho(Q(a+1, b, c))$ since $Q(a, b, c)$ is a proper subgraph of $Q(a+1, b, c)$. Note that $Q(a+1, b, c)$ is obtained from $Q(a+1, b-1, c)$ by subdividing an edge on an internal path. So, by Lemma 2 we have $\rho(Q(a+1, b, c)) < \rho(Q(a+1, b-1, c))$. Then the desired inequality follows. It completes the proof of Theorem 2. \square

Theorem 3. For $k > 2$, there is an N such that when $n > N$ we have

$$\begin{aligned} \rho(T(1, 2, n-4)) &< \rho(Q(2, n-6, 3)) < \rho(Q(3, n-7, 3)) < \rho(T(1, 3, n-5)) \\ &< \rho(Q(2, n-7, 4)) < \rho(Q(3, n-8, 4)) < \rho(Q(4, n-9, 4)) \\ &< \rho(T(1, 4, n-6)) < \cdots < \rho(Q(k, n-2k-1, k)) < \rho(T(1, k, n-k-2)) \\ &< \rho(T(1, k+1, n-k-3)) < \rho(T(1, k+2, n-k-4)) \\ &< \cdots < \rho\left(T\left(1, \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right)\right) < \rho(T(2, 2, n-5)). \end{aligned}$$

Proof. The inequalities between $\rho(T(*, *, *))$'s and between $\rho(Q(*, *, *))$'s are directly from Theorems 1 and 2. The inequalities between $\rho(T(*, *, *))$ and $\rho(Q(*, *, *))$ are obtained from Lemma 5.

It completes the proof of Theorem 3. \square

For $k \geq 3$, let $n(k) = \min\{n: \rho(Q(k, n-2k-1, k)) < \rho(T(1, k, n-k-2))\}$. This gives a threshold function. A natural but difficult problem is to determine $n(k)$. By calculations with the software MATLAB we find $n(3) = 16$, $n(4) = 21$ and $n(5) = 25$. Then we immediately have the following

Corollary 1. For $n > 24$, we have

$$\begin{aligned} \rho(T(1, 2, n-4)) &< \rho(Q(2, n-6, 3)) < \rho(Q(3, n-7, 3)) < \rho(T(1, 3, n-5)) \\ &< \rho(Q(2, n-7, 4)) < \rho(Q(3, n-8, 4)) < \rho(Q(4, n-9, 4)) \\ &< \rho(T(1, 4, n-6)) < \rho(Q(2, n-8, 5)) < \rho(Q(3, n-9, 5)) \\ &< \rho(Q(4, n-10, 5)) < \rho(Q(5, n-11, 5)) < \rho(T(1, 5, n-7)). \end{aligned}$$

Clearly we can go further with the help of computer calculation. We conjecture that $n(k)$ is strictly increasing with k .

4. Application to acyclic Kekulean molecules with large HOMO–LUMO separation

The difference between the highest occupied molecular orbit and the lowest unoccupied molecular orbit, HOMO–LUMO separation, is well known to be an important parameter in chemistry. This parameter is equal to the difference between the least positive and greatest negative eigenvalues of a molecular graph. In this section we shall study the ordering for the acyclic Kekulean molecules with large HOMO–LUMO separation. The acyclic Kekulean molecules in chemistry correspond to the trees with perfect matching in graph theory. In this case the HOMO–LUMO separation is just twice the least positive eigenvalue, since the spectrum of such a tree (as a bipartite graph with an even number of vertices) is symmetric with respect to zero (see [1]).

For convenience we shall denote the least positive eigenvalue of a graph G as $\mu(G)$. Shao and Hong [18] determined the upper bound of $\mu(T)$ for the trees T with perfect matching and determined the unique tree with its least positive eigenvalue reaching the upper bound. Zhang and Chang [21] further determined the trees T with $\mu(T)$ to be the second largest and the third largest. In this section we shall determine the trees T with $\mu(T) > \frac{1}{2}(\sqrt{6} + \sqrt{5} - \sqrt{2} + \sqrt{5}) \approx 0.4058$ and give an asymptotic ordering. It should be pointed out that the family of these trees is infinite.

We need some definitions and results from [18].

Definition 1. Let Γ_{2n} be the set of trees each of which has order $2n$ and has exactly n vertices with degree equal to 1 and these n vertices have n distinct neighbors.

Definition 2. For $T \in \Gamma_{2n}$, the subgraph obtained from T by deleting the n vertices of degree 1 and the n pendant edges is called the contracted subtree of T and denoted as \hat{T} .

Note that for $T \in \Gamma_{2n}$, \hat{T} is a tree with n vertices. On the other hand, for any tree T of order n , the new tree of order $2n$ obtained by attaching a new pendant edge to each vertex of T is called the *expanded tree* of T and denoted as \tilde{T} .

Clearly, $\tilde{T} \in \Gamma_{2n}$ for any tree T of order n . It is also clear that if $T \in \Gamma_{2n}$ then $\tilde{\tilde{T}} = T$.

Lemma 7 (see Zhang and Chang [21, Lemma 2]). For $T \in \Gamma_{2n}$, the least positive eigenvalue of T is $\lambda_n(T) = \frac{1}{2}(\sqrt{\rho^2(\hat{T}) + 4} - \rho(\hat{T}))$.

(We note that the proof of this lemma given in [21] contains an error in its lines 5 and 6, which should be corrected by changing to the following:

“So the positive eigenvalues of T are $\frac{1}{2}(\sqrt{x_i^2(\hat{T}) + 4} + x_i(\hat{T}))$, $i = 1, 2, \dots, k$. Since $f(x) = \frac{1}{2}(\sqrt{x^2 + 4} + x)$ is an increasing function of x , and the minimum eigenvalue of \hat{T} is $x_k(\hat{T}) = -x_1(\hat{T})$, we see that the k th largest eigenvalue”.)

Lemma 8 (Shao and Hong [18]). Let \mathcal{T}_{2n} denote the set of all trees with order $2n$, and let $a_n = \max\{\lambda_n(T) : T \in \mathcal{T}_{2n} - \Gamma_{2n}\}$. Then $a_{n-1} \geq a_n$, $n = 2, 3, \dots$.

Theorem 4. For $n \geq 6$, let

$$\mathcal{U}_{2n} = \{T : T \in \mathcal{T}_{2n}, \lambda_n(T) > \frac{1}{2}(\sqrt{6 + \sqrt{5}} - \sqrt{2 + \sqrt{5}})\}.$$

Then $\mathcal{U}_{2n} = \{\tilde{T} : T \in \Omega_1 \cup \Omega_2\}$.

Proof. By computer calculation we have $a_6 \approx 0.4038 \geq a_7 \geq a_8 \geq \dots$. For $T \in \mathcal{U}_{2n}$, by definition we have $\lambda_n(T) > \frac{1}{2}(\sqrt{6 + \sqrt{5}} - \sqrt{2 + \sqrt{5}}) \approx 0.4058$. So $\mathcal{U}_{2n} \subseteq \Gamma_{2n}$. Note that the function $f(x) = \frac{1}{2}(\sqrt{x^2 + 4} - x)$ is a decreasing function of x and that $f(x) = \frac{1}{2}(\sqrt{6 + \sqrt{5}} - \sqrt{2 + \sqrt{5}})$ when $x = \sqrt{2 + \sqrt{5}}$. So, by Lemma 7, we see that $\lambda_n(T) > \frac{1}{2}(\sqrt{6 + \sqrt{5}} - \sqrt{2 + \sqrt{5}})$ if and only if $\rho(\tilde{T}) < \sqrt{2 + \sqrt{5}}$.

Then, from Lemmas 3 and 4 we see that $\tilde{T} \in \Omega_1 \cup \Omega_2$. It completes the proof of Theorem 4. \square

Theorem 5. For $k > 2$, there is an N such that when $n > N$ we have

$$\begin{aligned} \lambda_n(\tilde{P}_n) &> \lambda_n(\tilde{Z}_n) > \lambda_n(\tilde{W}_n) > \lambda_n(\tilde{T}(1, 2, n-4)) > \lambda_n(\tilde{Q}(2, n-6, 3)) \\ &> \lambda_n(\tilde{Q}(3, n-7, 3)) > \lambda_n(\tilde{T}(1, 3, n-5)) > \lambda_n(\tilde{Q}(2, n-7, 4)) \\ &> \lambda_n(\tilde{Q}(3, n-8, 4)) > \lambda_n(\tilde{Q}(4, n-9, 4)) > \lambda_n(\tilde{T}(1, 4, n-6)) \\ &> \dots > \lambda_n(\tilde{Q}(k, n-2k-1, k)) > \lambda_n(\tilde{T}(1, k, n-k-2)) \\ &> \lambda_n(\tilde{T}(1, k+1, n-k-3)) > \lambda_n(\tilde{T}(1, k+2, n-k-4)) \\ &> \dots > \lambda_n\left(\tilde{T}\left(1, \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right)\right) > \lambda_n(\tilde{T}(2, 2, n-5)). \end{aligned}$$

Proof. By Lemma 7, we see that for any $H, K \in \Gamma_{2n}$, $\lambda_n(H) < \lambda_n(K)$ when $\rho(\hat{H}) > \rho(\hat{K})$. So, the inequalities in Theorem 5 can be easily obtained from Theorem 3 and the inequalities (*) in Section 3. \square

Corollary 2. For $n > 49$, we have

$$\begin{aligned} \lambda_n(\check{P}_n) &> \lambda_n(\check{Z}_n) > \lambda_n(\check{W}_n) > \lambda_n(\check{T}(1, 2, n-4)) > \lambda_n(\check{Q}(2, n-6, 3)) \\ &> \lambda_n(\check{Q}(3, n-7, 3)) > \lambda_n(\check{T}(1, 3, n-5)) > \lambda_n(\check{Q}(2, n-7, 4)) \\ &> \lambda_n(\check{Q}(3, n-8, 4)) > \lambda_n(\check{Q}(4, n-9, 4)) > \lambda_n(\check{T}(1, 4, n-6)) \\ &> \lambda_n(\check{Q}(2, n-8, 5)) > \lambda_n(\check{Q}(3, n-9, 5)) > \lambda_n(\check{Q}(4, n-10, 5)) \\ &> \lambda_n(\check{Q}(5, n-11, 5)) > \lambda_n(\check{T}(1, 5, n-7)). \end{aligned}$$

It is clear that we can go further as we pointed out after Corollary 1.

Acknowledgements

The authors would like to thank the referees for their helpful comments and suggestions.

References

- [1] N. Biggs, Algebraic Graph Theory, Cambridge University Press, Cambridge, 1974, 1993.
- [2] A.E. Brouwer, A. Neumaier, The graph with spectral radius between 2 and $\sqrt{2 + \sqrt{5}}$, Linear Algebra Appl. 114/115 (1989) 273–276.
- [3] F.R.K. Chung, Spectral Graph Theory, American Mathematical Society, Rhode Island, 1997.
- [4] L. Collatz, U. Sinogowitz, Spektren endlicher Grafen, Abh. Math. Sem. Univ. Habary 21 (1957) 63–77.
- [5] D.M. Cvetković, M. Doob, I. Gutman, On graphs whose eigenvalues do not exceed $\sqrt{2 + \sqrt{5}}$, Ars Combin. 14 (1982) 225–239.
- [6] D.M. Cvetković, M. Doob, I. Gutman, A. Torgasev, Recent Results in the Theory of Graph Spectra, North-Holland, Amsterdam, 1988.
- [7] D.M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs, Academic Press, New York, 1980. Third edition, Johann Ambrosius, Barth, Verlag 1995.
- [8] D.M. Cvetković, I. Gutman, On the spectral structure of graphs having the maximal eigenvalue not greater than 2, Publ. Inst. Math. (Beograd) 18 (1975) 39–45.
- [9] D.M. Cvetković, P. Rowlinson, The largest eigenvalue of graph: a survey, Linear Multilinear Algebra 28 (1990) 3–33.
- [10] D.M. Cvetković, P. Rowlinson, S. Simić, Eigenspaces of Graphs, Cambridge University Press, Cambridge, 1997.
- [11] F. Goodman, P. de la Harpe, V. Jones, Matrices over natural numbers: values of norms, classification and variations in Dynkin Diagrams and Towers of Algebras, Report Univ. de Geneve, June 1986, Chapter 1.
- [12] A.J. Hoffman, On limit points of spectral radii of non-negative symmetric integral matrices, in: Y. Alavi et al. (Eds.), Graph Theory and its Application, Lecture Notes in Mathematics, Vol. 303, Springer, New York, 1972, pp. 165–172.
- [13] A.J. Hoffman, J.H. Smith, On the spectral radii of topologically equivalent graphs, in: M. Fiedler (Ed.), Recent Advances in Graph theory, Academia Praha, Prague, 1975, pp. 273–281.
- [14] M. Hofmeister, On the two largest eigenvalues of tree, Linear Algebra Appl. 260 (1997) 43–59.
- [15] Q. Li, K. Feng, On the largest eigenvalue of graphs (Chinese), Acta Math. Appl. Sinica 2 (1979) 167–175 (MR80k:05079).
- [16] L. Lovasz, J. Pelikan, On the eigenvalues of trees, Periodica Math. Hung. 3 (1973) 175–182.

- [17] P. Rowlinson, in: *Graph perturbations, Surveys in Combinatorics*, London Mathematical Society, Lecture Notes Series 166, Cambridge University Press, Cambridge, 1991.
- [18] J.Y. Shao, Y. Hong, Bound on the smallest positive eigenvalue of tree with perfect matching, *Chin. Sci. Bull. (English edition)* 37 (9) (1992) 713–717.
- [19] J.B. Shearer, On the distribution of the maximum eigenvalue of graphs, *Linear Algebra Appl.* 114/115 (1989) 17–20.
- [20] J.H. Smith, Some properties of the spectrum of a graph, in: R. Guy et al. (Eds.), *Combinatorial Structures and Their Applications*, Gordon and Breach, New York, London, Paris, 1970, pp. 403–406.
- [21] F.J. Zhang, A. Chang, Acyclic molecules with greatest HOMO–LUMO separation, *Discrete Appl. Math.* 98 (1999) 165–171.